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AN UPDATED VERSION OF THE KANTOROVICH THEOREM FOR NEWTON'S METHOD

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(6) AN UPDATED VERSION OF THE KANTOROVICH THEOREM FOR NEWTON'S METHOD.

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ABSTRACT (15) DAAG29-80-C-0041

An affine invariant version of the Kantorovich theorem for Newton's method is presented. The result includes the Gragg-Tapia error bounds, as well as recent optimal and sharper upper bounds, new optimal and sharper lower bounds, and new inequalities showing q-quadratic convergence all in terms of the usual majorizing sequence. Closed form expressions for these bounds are given.

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Key Words: Nonlinear equations, Newton method, Kantorovich theorem, Error bounds

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SIGNIFICANCE AND EXPLANATION

A basic problem in numerical analysis is the computation of the roots of a nonlinear system $Fx = 0$, where $F : X \to X$ and X is a space of N-tuples. Newton's method consists of the iteration,

$$x_0 \text{ chosen}, \quad x_n = x_{n-1} - F'(x_{n-1})^{-1}Fx_n, \quad n \geq 1 \quad ,$$

where $F'(x_{n-1})$ is the Jacobian of F at x_{n-1}, thus generating a sequence of N-tuples $x_n = (\xi_{n1}, \xi_{n2}, \ldots, \xi_{nN})$, which will hopefully converge to a solution $x^* = (\xi_1^*, \xi_2^*, \ldots, \xi_N^*)$. The basic idea of the method is to take each vector x_n as the solution of an approximating system of $N \times N$ linear equations. The Kantorovich theorem gives specific conditions under which the iterates x_n will converge to a solution x^*, establishing in the process the local existence and uniqueness of that solution, and it also yields computable upper and lower bounds for the errors $\|x^* - x_n\|$. For mathematical expediency, this famous theorem is often stated in terms of operator equations in Banach spaces, but its major application to actual computer work is restricted to finite systems of equations as described above. Although the theorem has been established conclusively in 1948, there is a continuing effort on the part of researchers to find the best possible and sharpest error bounds under the hypotheses of the theorem. In practice, when guaranteed accuracy is needed, error bounds provide exit criteria, viz., means of stopping the computation when an approximant has a prescribed accuracy. Thus the sharpness of error bounds is important, since it translates into saving of computer time. This report presents a complete update of the theorem, giving recent and new sharper error bounds.

The responsibility for the wording and views expressed in this descriptive summary lies with MRC, and not with the author of this report.

AN UPDATED VERSION OF THE KANTOROVICH THEOREM FOR NEWTON'S METHOD

George Miel†

Introduction. Kantorovich [5] presented in 1939 a preliminary convergence result for Newton's method. In 1948, he used certain recurrence relations to establish his now-famous thoerem [6], and a year later, he gave the first proof based on the majorant principle [7]. Various workers have presented refinements of the theorem and related results. For a survey of the theorem's predecessors and successors prior to 1970, see [2, p. 247], [15, pp. 420, 428], [16, p. 404].

With the use of the original recurrence relations, Dennis [1] improved the Kantorovich error bounds. Tapia [22] derived these improved bounds directly from Ortega's majorizing sequence [14]. Rall and Tapia [20] further improved the bounds. Under hypotheses different from the usual ones, Ostrowski [16], [17] established optimal a priori upper bounds. Gragg and Tapia [4] used the recurrence relations to get optimal a posteriori upper and lower bounds. Ptak [19] applied his principle of nondiscrete induction to derive the optimal a priori upper bounds. With the same principle, Potra and Pták [18] obtained a posteriori upper and lower bounds sharper than those of Gragg-Tapia. Miel [9], [10] used the majorizing sequence to derive the Gragg-Tapia upper bounds, as well as new optimal and sharper upper bounds. It turns out [11] that these new bounds are finer than those of Potra-Pták.

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Although the lasting effort that has gone into finding error bounds for the Kantorovich theorem is suggestive of the theorem's depth and its central importance in nonlinear numerical analysis, one cannot help yearn for a clean and definitive statement. Since recent refinements are either scattered or altogether not in the open literature, our purpose here is to give a complete update. As it should be, the updated theorem is affine invariant [3], and it describes clearly in terms of the usual majorizing sequence the Gragg-Tapia bounds, the recent optimal and sharper upper bounds, new optimal and finer lower bounds, and new inequalities showing q-quadratic convergence. Since the elements of the majorizing sequence are known in closed form, we readily get explicit expressions for all bounds.

Given a sequence $\{x_n\}_{n=0}^{\infty}$ in a Banach space, if there is a sequence of real numbers $\{t_n\}_{n=0}^{\infty}$ such that

$$\lim t_n = t^* < \infty, \quad \|x_n - x_{n-1}\| \leq t_n - t_{n-1} \quad , \tag{1.1}$$

then $\{x_n\}_{n=0}^{\infty}$ converges to some x^* and the error bounds

$$\|x^* - x_n\| \leq t^* - t_n \tag{1.2}$$

are valid [14]. The following simple result [10], given here for completeness, shows that under certain conditions, the majorizing sequence $\{t_n\}_{n=0}^{\infty}$ yields error bounds much sharper than (1.2).

LEMMA. If there is a sequence $\{t_n\}_{n=0}^{\infty}$ of real numbers such that (1.1) hold and

$$t_0 = 0, \quad t_{n-1} < t_n, \quad \|x_{n+1} - x_n\| \leq \frac{t_{n+1} - t_n}{(t_n - t_{n-1})^2} \|x_n - x_{n-1}\|^2 \quad ,$$

then $\{x_n\}_{n=0}^{\infty}$ converges to some x^* and

$$(1.3)\qquad \|x^* - x_n\| \le \frac{t^* - t_n}{(t_n - t_{n-1})^2}\|x_n - x_{n-1}\|^2 \le \frac{t^* - t_n}{t_n - t_{n-1}}\|x_n - x_{n-1}\|$$

$$\le \frac{t^* - t_n}{t_1}\|x_1 - x_0\| \quad .$$

Proof. If $m > n$ then

$$\|\nabla x_m\| \le \nabla t_m \left(\frac{\|\nabla x_n\|}{\nabla t_n}\right)^{2^{m-n}} \le \nabla t_m \left(\frac{\|\nabla x_n\|}{\nabla t_n}\right)^2 \quad .$$

Thus for $p \geq 1$,

$$\|x_{n+p} - x_n\| \le (t_{n+p} - t_n)\left(\frac{\|\nabla x_n\|}{\nabla t_n}\right)^2 \quad .$$

Take $p \to \infty$ to obtain the first inequality in (1.3). Finally, use $\|\nabla x_n\|/\nabla t_n \le \|\nabla x_1\|/t_1 \le 1$ to get the other two inequalities.

Given Newton iterates for an operator equation $Gx = 0$,

$$(1.4)\qquad x_{n+1} = x_n - G'(x_n)^{-1}Gx_n \quad ,$$

the usual majorizing sequence consists of the scalar Newton iterates,

$$(1.5)\qquad t_0 = 0, \quad t_{n+1} = t_n - g'(t_n)^{-1}g(t_n) \quad ,$$

of a quadratic polynomial $g(t)$ whose coefficients depend on G and x_0. Since g satisfies the Kantorovich hyptheses and (1.5) then is a special case of (1.4) with $G = g$ and $x_0 = t_0$, the bounds in (1.2) and (1.3) are all

optimal. A standard argument and the bounds $\|G'(x_n)^{-1}\| \leq -g'(t_n)^{-1}$ yield a quadratic inequality, (2.5) in the sequel, from which one gets lower bounds for $\|x^* - x_n\|$ in terms of $\|x_{n+1} - x_n\|$. The weaker optimality of these lower bounds is obtained as in Gragg-Tapia [4].

Warnings against the use of majorizing sequences are sometimes sounded. The reasons given are the apparent r-order of convergence, the coarseness of the bounds, and the difficulty in computing the required constants. The arguments against majorizing sequences should perhaps be re-evaluated, since the updated theorem shows that the majorizing sequence does imply q-quadratic convergence and that new error bounds are sharper than the usual ones. The problems associated with the local nature of the estimates and the verification of hypotheses, however, do remain. In this connection, we point to research on computer verification of semilocal conditions by interval analysis and on interval versions of Newton's method [12], [13], [21].

2. The Updated Theorem. Let X and Y be Banach spaces and let D be an open convex subset of X. The open ball $\{x : \|x - x_0\| < r\}$ and its closure are denoted by $S(x_0,r)$ and $\bar{S}(x_0,r)$ respectively.

THEOREM. Let $F : D \quad X \to Y$ be Fréchet differentiable. Assume that $F'(x_0)$ is invertible for some $x_0 \in D$, and that

$$\|F'(x_0)^{-1}(F'(x) - F'(y))\| \leq K\|x - y\|, \quad x,y \in D \quad ,$$

$$\|F'(x_0)^{-1}Fx_0\| \leq a \quad ,$$

$$S(x_0,t^*) \subset D, \quad t^* = (1 - \sqrt{1 - h})/K, \quad h = 2Ka \leq 1 \quad .$$

Consider the scalar iterates (1.5) for the quadratic polynomial $g(t) = \frac{K}{2} t^2 - t + a$. Then

i) The iterates $x_{n+1} = x_n - F'(x_n)^{-1}Fx_n$ exist, remain in $S(x_0,t^*)$, and converge to a root x^* of F.

ii) The root x^* is unique in $S(x_0,t^{**}) \cap D$, $t^{**} = (1 + \sqrt{1 - h})/K$, if $h < 1$, and in $\bar{S}(x_0,t^{**})$ if $h = 1$.

iii) The upper error bounds (1.3) are valid.

iv) $$\frac{2\|x_{n+1} - x_n\|}{1 + \sqrt{1 + 4\left(\dfrac{t_{n+1} - t_n}{t_n - t_{n-1}}\right)^2}} \leq \frac{2\|x_{n+1} - x_n\|}{1 + \sqrt{1 + 4\dfrac{(t^* - t_{n+1})}{(t^* - t_n)^2}\|x_{n+1} - x_n\|}}$$

$$\leq \|x^* - x_n\| \quad .$$

v) $$\|x^* - x_{n+1}\| \leq \frac{t^* - t_{n+1}}{(t^* - t_n)^2}\|x^* - x_n\|^2 \quad .$$

Also, the uniqueness statement (ii) and the bounds in (iii), (iv), and (v) are best possible.

Proof. Consider the scaling,

$$Gx = F'(x_0)^{-1}Fx \quad . \tag{2.1}$$

The Banach lemma implies that $G'(x)$ is invertible for every $x \varepsilon S(x_0,t^*)$. If both x and $Hx = x - G'(x)^{-1}Gx$ are in $S(x_0,t^*)$ then

$$\|H(Hx) - Hx\| \leq \frac{K/2}{1 - K\|Hx - x_0\|} \|Hx - x\|^2 \quad .$$

The sequence $\{t_n\}$ satisfies the conditions $\|x_1 - x_0\| \leq t_1 = a$, $t_{n-1} < t_n$, $\lim t_n = t^*$, and

$$\frac{K/2}{1 - Kt_n} = \frac{t_{n+1} - t_n}{(t_n - t_{n-1})^2} \quad . \tag{2.2}$$

An induction argument shows that $\{x_n\}$ exists in $S(x_0,t^*)$ and that the hypotheses of the lemma hold. We thus get (i) and (iii). Consideration of the simplified Newton method yields (ii). Letting $e_n = t^* - t_n$, we have

$$e_0 = t^*, \quad e_{n+1} = \frac{e_n^2}{2e_n + \Delta}, \quad \Delta = t^{**} - t^* \quad , \tag{2.3}$$

$$\|G'(x_n)^{-1}\| \leq -g'(t_n)^{-1} = \frac{1}{1 - Kt_n} = \frac{2}{K} \cdot \frac{e_{n+1}}{e_n^2} \quad . \tag{2.4}$$

From the identity

$$x_{n+1} - x_n = (x^* - x_n) + G'(x_n)^{-1}(Gx^* - Gx_n - G'(x_n)(x^* - x_n)) \quad ,$$

a mean-value theorem, and (2.4), we get

$$(2.5) \qquad \frac{e_{n+1}}{e_n^2}\|x^* - x_n\|^2 + \|x^* - x_n\| - \|x_{n+1} - x_n\| \geq 0 \quad .$$

The sharper lower bounds in (iv) follow. Use $\|x_{n+1} - x_n\| \leq t_{n+1} - t_n$ and

$$\frac{e_{n+1}}{e_n^2} = \frac{t_{n+1} - t_n}{(t_n - t_{n-1})^2} ,$$

which results from (2.2) and (2.4), to get the other lower bounds. Use (2.4) and a mean-value theoren on

$$\|x^* - x_{n+1}\| \leq \|G'(x_n)^{-1}\| \; \|Gx^* - Gx_n - G'(x_n)(x^* - x_n)\|$$

to get (v). Obtain the optimality as indicated in the introduction to complete the proof.

The bounds in the theorem are expressed in terms of the majorizing sequence, but since Newton iterates for quadratic polynomials are known in closed form, [8, p. 28] or [17, Appendix F], these bounds can be given explicitly.

COROLLARY. Assume that the hypotheses of the theorem hold and let $\Delta = t^{**} - t^*$ and $\theta = t^*/t^{**}$. Then

$$\frac{2\|x_{n+1} - x_n\|}{1 + \sqrt{1 + \dfrac{4\theta^{2^n}}{(1 + \theta^{2^n})^2}}} \leq \frac{2\|x_{n+1} - x_n\|}{1 + \sqrt{1 + \dfrac{4}{\Delta}\,\dfrac{1 - \theta^{2^n}}{1 + \theta^{2^n}}\,\|x_{n+1} - x_n\|}} \leq \|x^* - x_n\| \leq$$

$$\frac{1 - \theta^{2^n}}{\Delta}\|x_n - x_{n-1}\|^2 \leq \theta^{2^{n-1}}\|x_n - x_{n-1}\| \leq \frac{\Delta\theta^{2^n}}{a(1 - \theta^{2^n})} \cdot \|x_1 - x_0\|$$

if $h < 1$, and

$$2(\sqrt{2}-1)\|x_{n+1}-x_n\| \le 2^{-n+1}a\left(\sqrt{1+\frac{2^n}{a}\|x_{n+1}-x_n\|}-1\right) \le \|x^*-x_n\| \le$$

$$\frac{2^{n-1}}{a}\|x_n-x_{n-1}\|^2 \le \|x_n-x_{n-1}\| \le 2^{-n+1}\|x_1-x_0\|$$

if $h = 1$.

Proof. We first solve the nonlinear difference equation (2.3). If $h = 1$ then $\Delta = 0$ and

$$e_n = 2^{-n+1}a \quad . \tag{2.6}$$

If $h < 1$, let $u_n = e_n/(e_n + \Delta)$, thus getting $u_0 = \theta$, $u_{n+1} = u_n^2$. The solution is $u_n = \theta^{2^n}$, and so,

$$e_n = \frac{\Delta\theta^{2^n}}{1-\theta^{2^n}} \quad , \tag{2.7}$$

for $h < 1$. Now use (2.6) and (2.7) on

$$\left(\frac{t_{n+1}-t_n}{t_n-t_{n-1}}\right)^2 = \left(\frac{e_n-e_{n+1}}{e_{n-1}-e_n}\right)^2, \quad \frac{t^*-t_n}{(t_n-t_{n-1})^2} = \frac{e_n}{(e_{n-1}-e_n)^2} =$$

$$\frac{1}{e_n+\Delta}, \quad \text{etc.,}$$

to obtain the desired expressions.

3. Remarks and Numerical Example. We point out features of the above version of the Kantorovich theorem.

3.1. The theorem is affine invariant and the transformation (2.1) is an optimal scaling [3].

3.2. Statement (iv) gives an improvement of the Gragg-Tapia lower bounds, since the latter are equivalent to the left-most bounds.

3.3. The inequalities in (v) show that the majorizing sequence yields not only second r-order convergence, but the stronger second q-order as well. Indeed, if $h < 1$ then (2.3) implies that $\lim e_{n+1}/e_n^2 = 1/\Delta < \infty$.

3.4. The two right-most bounds in (1.3) are equivalent to the upper bounds of Gragg-Tapia. The bounds with $\|x_n - x_{n-1}\|^2$ are in practice considerably sharper.

3.5. The recent bounds of Potra-Pták [18], obtained by nondiscrete induction, become in our notation,

$$\gamma(\Delta/2,\ d_{n+1}) \leq \|x^* - x_n\| \leq \delta(\Delta/2,\ d_n), \qquad d_n = \|x_n - x_{n-1}\| ,$$

$$\gamma(s,t) = (s^2 + 4t^2 + 4t(s^2 + t^2)^{1/2})^{1/2} - (t + (s^2 + t^2)^{1/2}) ,$$

$$\delta(s,t) = (s^2 + t^2)^{1/2} - s .$$

These bounds are sharper than those of Gragg-Tapia. However, it turns out that $(t^* - t_n)d_n^2/(t_n - t_{n-1})^2 \leq \delta(\Delta/2,\ d_n)$, see [11]. Numerical experiments also indicate that the sharper lower bounds in (iv) are finer than $\gamma(\Delta/2,\ d_{n+1})$.

3.6. In practice, the user should employ the sharpest bounds,

$$\frac{2d_{n+1}}{1 + \sqrt{1 + 4a_n d_{n+1}}} \leq \|x^* - x_n\| \leq A_n d_n^2 . \tag{3.1}$$

The following recurrence relations are convenient for programmed computation:

$$(3.2) \qquad a_0 = (t^* + t^{**})^{-1}, \quad a_{n+1} = \frac{2a_n}{1 + \Delta^2 a_n^2},$$

$$(3.3) \qquad A_1 = \theta/a, \quad A_{n+1} = A_n(2 - \Delta A_n) .$$

Use (2.3) and $a_n = 1/(2e_n + \Delta)$ to verify (3.2). For (3.3), see [10, p. 192].

3.7. We borrow an example given in [18]. The table lists all the bounds stated in the theorem for the scalar cubic $F(x) = \frac{1}{3}(x^3 - 1)$, with $x_0 = 1.3$, $a = 0.236095$, $K = 0.209727$. The bounds in (3.1), especially the upper bounds, are seen to be sharper.

TABLE

$$g(t) = 0.1048632758\, t^2 - t + 0.2360946746$$

$$t^* = 0.4298664530 \qquad t^{**} = 0.5237562515$$

n	$\dfrac{2d_{n+1}}{1+\sqrt{1+4\left(\dfrac{t_{n+1}-t_n}{t_n-t_{n-1}}\right)^2}}$	$\dfrac{2d_{n+1}}{1+\sqrt{1+4\dfrac{(t^*-t_{n+1})}{(t^*-t_n)^2}d_{n+1}}}$	x_n	$\dfrac{t^*-t_n}{(t_n-t_{n-1})^2}\cdot d_n^2$	$\dfrac{t^*-t_n}{t_n-t_{n-1}}\cdot d_n$	$\dfrac{t^*-t_n}{t_1}\, d_1$
0	.1958656190	.2152158729	1.3000000000			
1	.0501050050	.0571992421	1.0639053254	.1937717784	.1937717784	.1937717784
2	.0031714276	.0037228786	1.0037617275	.0210451135	.0405133423	.0779910692
3	.0000125068	.0000140791	1.0000140800	.0001187900	.0017004978	.0243428972
4	.0000000002	.0000000002	1.0000000002	.0000000020	.0000028989	.0041562278

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An affine invariant version of the Kantorovich theorem for Newton's method is presented. The result includes the Gragg-Tapia error bounds, as well as recent optimal and sharper upper bounds, new optimal and sharper lower bounds, and new inequalities showing q-quadratic convergence all in terms of the usual majorizing sequence. Closed form expressions for these bounds are given.